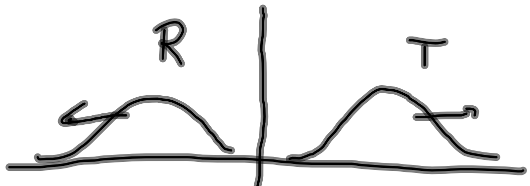
1 D Scattering : $H = -\frac{1}{2}\frac{d^2}{dx^2} + V_0 \operatorname{sech}^2(\overset{\alpha x}{x})$

$" \frac{1}{\cosh^2(x\alpha)}$

For a given V_0, find the transmission coeff. as a fct of $E = \frac{1}{2}k^2$



$T = \frac{\sum |\psi_T|^2}{\sum |\psi_0|^2}$

Sum R $= \sum |\psi_R|^2$

Sum T $= \sum |\psi_T|^2$

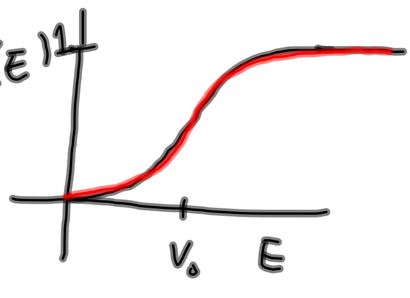
Total $=$ Sum R $+$ Sum T

$E_0 = \frac{1}{2}k_0^2$ then $T = \frac{1}{1 + \cosh^2\left(\pi\sqrt{2V_0 - 1/4}\right) / \sinh^2(\pi k_0)}$

choose $V_0 = 48.2$ if $E_0 = V_0$

$T = 0.520001$

for project compute $T(E)$



Higher order algorithms – splitting algorithm

$e^{\epsilon(T+V)}$ ← classical dynamics $\epsilon = \text{real}$ ✓
quantum " $\epsilon = -i\delta t$ ✓
← quantum statistical mechanics $\epsilon = -\tau$ ✓

$\langle x' | e^{-\tau(T+V)} | x \rangle$ = density matrix

$Z = \int dx \, \langle x | e^{-\tau(T+V)} | x \rangle$

Second order: $e^{\epsilon(T+V)} \sim e^{\frac{1}{2}\epsilon V} e^{\epsilon T} e^{\frac{1}{2}\epsilon V} = T_2(\epsilon)$

The simplest 4^{th} order = Forest-Ruth

$T_2(\tilde{\epsilon})\, T(s\tilde{\epsilon})\, T_2(\tilde{\epsilon})$ has large error

$\tilde{\epsilon} = \frac{\epsilon}{2-s}$ $s = 2^{1/3}$ negative time step.

OK for class. Dyn + Q. Mech.
but NOT for Q. Stat. Mech $\sim e^{\epsilon \nabla^2}$
cannot have negative time steps $e^{-\tau(-\frac{1}{2}\nabla^2)} \sim e^{\tau \nabla^2}$ diffusion operator
can't do diffusion backward in time.

Sheng-Suzuki Thm can't have positive time steps beyond second order.

$$e^{\epsilon(T+V)} = \prod_{i=1}^{N} e^{a_i \epsilon T} e^{b_i \epsilon V}$$

i.e. $\{a_i, b_i\}$ can't all be positive beyond second order

Forward algorithm → only positive $\{a_i, b_i\}$
if in additional to T, V $T = -\frac{1}{2}\nabla^2$
keep another operator $V = V(r)$

$e^{\epsilon(T+V)}$ $[V,[T,V]] = |\vec{\nabla} V|^2 = \underbrace{\sum_{i=1}^{3} (\nabla_i V)^2}$ an additional potential

$$T_A^{(4)}(\epsilon) = e^{\frac{1}{6}\epsilon V} e^{\frac{1}{2}\epsilon T} e^{\frac{2}{3}\epsilon \tilde{V}} e^{\frac{1}{2}\epsilon T} e^{\frac{1}{6}\epsilon V} + O(\epsilon^5)$$

$$\tilde{V} = V + \frac{1}{48}\epsilon^2 [V,[T,V]]$$

$$T_A^{(4)}(\epsilon) = e^{\epsilon(T+V)} + O(\epsilon^5)$$